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What are 'good' points for local interpolation by radial basis functions?

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Abstract

Radial basis function interpolation has an advantage over other methods in that the interpolation matrix is nonsingular under very weak conditions on the location of the interpolation points. However, we show that point location can have a significant effect on the performance of an approximation in certain cases. Specifically, we consider multiquadric and thin plate spline interpolation to small data sets where derivative estimates are required. Approximations of this type are important in the motion of unsteady interfaces in fluid dynamics. For data points in the plane, it is shown that interpolation to data on a circle can be related to the polynomial case. For scattered data on the sphere, a comparison is made with the results of Sloan and Womersley.

1 Introduction

Radial basis functions (RBFs) such as multiquadrics or thin plate splines have been successfuly used for scattered data approximation in many applications. They have been shown to perform well for data fitting, although problems of ill-conditioning and the computational cost of processing large data sets must be handled carefully. In general, when considering the accuracy of a RBF interpolant, a balance must be achieved between the reduction in fill distance necessary for convergence of the approximation to an assumed underlying function and the need to maximise the separation distance between data points to avoid problems of ill-conditioning [4].

In the present study, we focus on the use of RBF approximation as one stage of a larger algorithm to compute the evolution of an unsteady interface in fluid dynamics. The accuracy of the approximations made in the algorithm and the interaction between its different stages determine whether the output is close to the true solution of the governing equations or whether spurious effects are produced. In the three-dimensional setting, a typical example is described by Zinchenko *et al.* [8] where the deformation of liquid drops in a viscous medium is studied. A critical feature of the algorithm is the approximation of the normal directions and curvatures of the droplet surface defined at a number of discrete points.

The focus here is algorithmic rather than theoretical and we investigate the performance of multiquadric and thin plate spline local interpolants applied to the determination of normal directions and curvatures of a smooth, closed surface. Certain configurations of data points, such as points located on a circle, impose constraints on the interpolant. A framework for understanding the behaviour of the RBF interpolants is provided by a comparison with the multivariate polynomial interpolant of de Boor and Ron [1] and by considering the free parameter in the multiquadric as a tensioning parameter [2].

2 Approximation method

A common approach to solving fluid dynamics problems that include moving interfaces, combines a computational grid with meshless approximation methods. The governing partial differential equations, or corresponding integral equation formulation, are solved on the grid, while quantities characterising the interface are computed as meshless scattered data approximations.

Here we examine the behaviour of local RBF approximations in the general context described by Zinchenko *et al.* [8]. For a given data set, a particular point is selected together with its nearest neighbours giving a set of typically 6 or 7 points. The initial locations of these points may be determined by a regular mesh, but the surface is allowed to deform so that the approximation is essentially to a small set of scattered data. The constructed RBF interpolant, S, can be expressed as

$$S(x) = \sum_{j=1}^{N} a_j \phi(||x - x_j||) + \sum_{i=1}^{K} b_i p_i(x),$$

with the constraint

$$\sum_{j=1}^{N} a_j p_i(x_j) = 0, \qquad \text{for } 1 \leq i \leq K,$$

where $x \in \Re^2$ and $\{p_i(x)\}_{i=1:K}$ is a basis for the space of bivariate polynomials of degree $\leq m-1$ with $K = m(m+1)/2$. The chosen forms for ϕ are the thin plate spline

$$\phi(||x - x_j||) = ||x - x_j||^2 \log ||x - x_j||, \qquad \text{(TPS)}$$

and the multiquadric

$$\phi(||x - x_j||) = (||x - x_j||^2 + c^2)^{\frac{1}{2}}, \qquad \text{(MQ)}$$

with $||\cdot||$ taken to be the Euclidean norm.

A framework for interpreting the computed results in the context being considered can be derived from [2] where the arbitrary parameter, c, of the MQ function is viewed as a tensioning parameter. As $c \to \infty$ the MQ interpolant approaches the corresponding polynomial interpolant to the given data, while as $c \to 0$, the MQ surface is tensioned. Multivariate polynomial interpolation can fail on particular point sets and this has provided a motivation for using RBF methods. However, the algorithm of de Boor and Ron [1] provides a reliable means of computing the 'least' polynomial interpolant. This algorithm is used to compute a polynomial fit as one reference point for the interpretation of the MQ interpolants. A second reference point is provided by the TPS interpolant which gives a minimum energy surface in a certain norm. This is shown to correspond closely to the MQ fit for a 'small', but nonzero value of c. The MQ interpolant can thus be shown to connect the minimum energy, tensioned, TPS surface with the polynomial fit to given data as c increases. In a fluid dynamics context a fluid–fluid interface is often assumed to be represented by a C^∞ function (although cusps may occur requiring a change in the representation). This would suggest that a high degree polynomial would be preferred to a TPS surface.

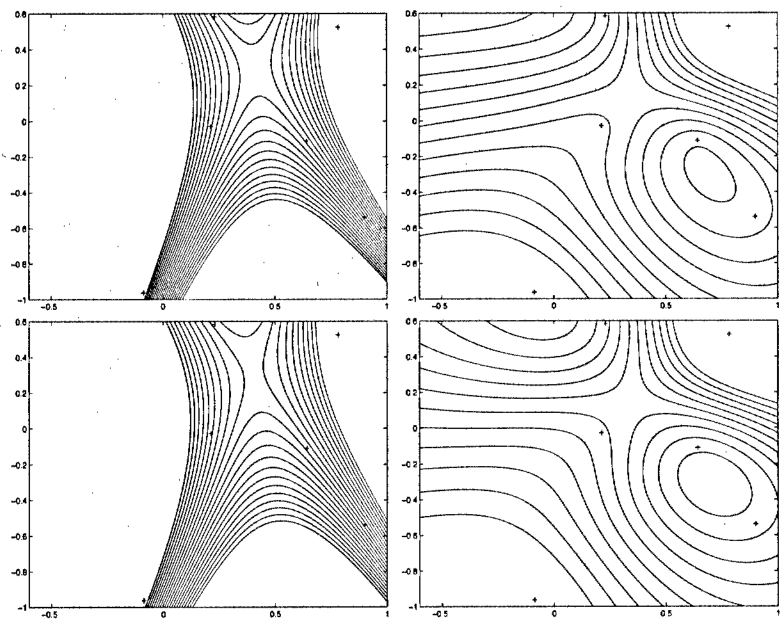

FIG. 1. Interpolants to random data at 6 points (+) in the plane: (left) polynomial (upper) and multiquadric (c = 10) (lower), contours [0:0.1:2]; (right) thin plate spline (upper) and multiquadric (c = 0.4) (lower), contours [0:0.1:1.1].

3 Scattered data in the plane

To illustrate the behaviour of local interpolation by MQ and TPS methods, random points in the xy-plane (with $-1 < x_i, y_i < 1$, for $i = 1:6$) are associated with random data values, f_i $(-1 < f_i < 1)$. Figure 1 shows, in the upper frames, the two reference

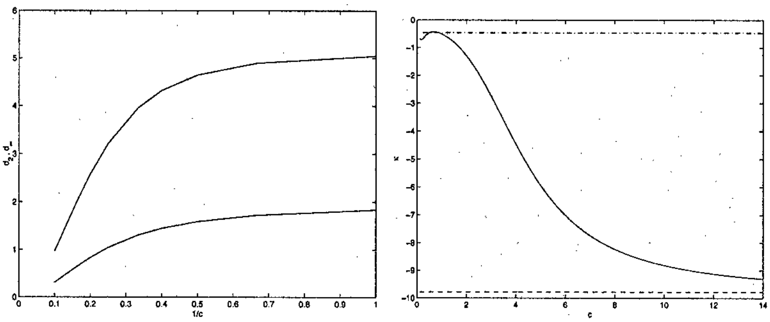

FIG. 2. Effect of varying the parameter c on multiquadric interpolants to random data in the plane: (left) norms of the difference between multiquadric and polynomial interpolants (upper curve $d_\infty = ||.||_\infty$, lower curve $d_2 = ||.||_2/\sqrt{N}$); (right) curvature ($\kappa = 2H$) computed at the centroid: — multiquadric; $- \cdot -$ thin plate spline; $--$ polynomial.

interpolating surfaces: (left) the polynomial surface computed by the algorithm of [1] and (right) the TPS surface. The lower frames give the contours of the MQ interpolants for $c = 10.0$ (left) and $c = 0.4$ (right). There is a close correspondence between the upper and lower frames on each side, but a large difference between the polynomial and TPS surfaces.

Figure 2 (left) shows the difference between the MQ surface and the polynomial reference interpolant computed on a regular grid on the interior of the circle with centre at the centroid of the data points $(0.44, -0.09)$ and radius the maximum distance from the centroid to a data point. There is convergence of the MQ surface to the polynomial as $1/c \to 0$, but the condition number of the interpolation matrix increases until the calculation cannot be continued. For $c = 10.0$ the condition number is 3×10^7.

As an indication of the behaviour of first and second partial derivatives of the interpolating surfaces we calculate the curvature at the centroid of the data points for the polynomial and TPS, together with MQ as c varies, using $\kappa = 2H$ where H is the mean curvature. Figure 2 (right) shows that κ_{MQ} for the MQ interpolant coincides with the value $\kappa_{TPS} = -0.46$ for the TPS when $c \approx 0.4$. When $c < 0.4$, $\kappa_{MQ} < \kappa_{TPS}$, while $\kappa_{MQ} \to \kappa_P = -9.78$, the polynomial curvature, as c increases.

An interesting example is presented in [1] of polynomial interpolation for points located at the vertices of a regular hexagon

$$(x_i, y_i) = \left(\cos\left(\frac{2\pi i}{6}\right), \sin\left(\frac{2\pi i}{6}\right)\right), \qquad i = 1, \ldots, 6 \tag{3.1}$$

with data values $f_i = (-1)^i$. This gives the interpolant

$$p(x, y) = x^3 - 3xy^2. \tag{3.2}$$

Since the points lie on the unit circle, the quadratic polynomial

$$p_2(x, y) = 1 - x^2 - y^2$$

vanishes at the data points and this causes difficulties for general polynomial methods. MQ interpolants do not suffer from these difficulties. When $c = 10.0$, the MQ surface is very close to (3.2). As c becomes smaller, the MQ surface approaches that of the TPS with the data values becoming local maxima or minima as the surface is tensioned. In addition, the restriction of the data points to a circle implies that the interpolating polynomial is harmonic, but the convergence of the approximation is only first order [1]. The MQ surface for large c inherits the properties of the polynomial fit. Thus, points on a circle are 'good' if the data being interpolated correspond to a harmonic function, but 'bad' if the data describe a function which has a maximum or minimum within the circle or a singularity. These constraints on the interpolant are discussed further in Section 5.

4 Scattered data on the sphere

In this section we examine the accuracy obtained from three separate methods for interpolating scattered data on the unit sphere $S^2 \subset \Re^3$. In particular we compare the results obtained using the MQ basis function in $\Re^3$ with those obtained using the spherical harmonics of Sloan and Womersley[1] [6] and the C^1 Hermite interpolant of Renka [5]. For the multiquadric function, we list the uniform norm interpolation errors calculated using a range of values for the shape parameter c.

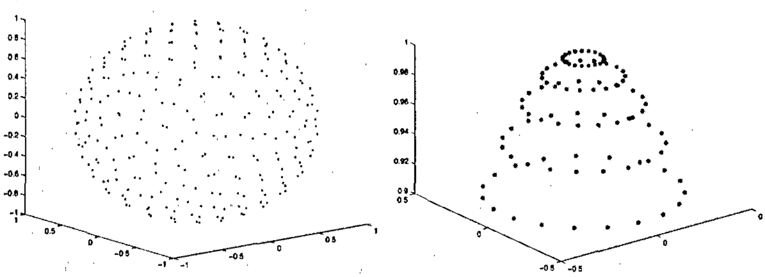

FIG. 3. Minimum energy points and spherical cap.

The point distribution used is the 256 'minimum energy' points of Fliege and Maier [3] and the uniform norm interpolation errors are calculated at points distributed on a spherical cap (see [5]).

The following functions are used for the comparisons in Table 4, where the results presented in [7] are labelled 'W&S'.

$$\begin{aligned} F1 &= \tfrac{1}{10}e^{x+y+z}, & F2 &= -5\sin(1+10z), \\ F3 &= \|\mathbf{x}\|_1/10, & F4 &= \sin^2(1+\|\mathbf{x}\|_1)/10. \end{aligned}$$

We note from Table 4 that the multiquadric function provides consistently better interpolants to the four test functions compared with the spherical harmonics. Here, the

[1]Uniform norm errors used for comparison are approximate only and were taken from graphical representations presented in Womersley and Sloan [7].

Method	F1	F2	F3	F4
W & S	2.0000e-10	0.5000	0.1100	0.0500
Renka	0.0013	0.1951	0.0054	0.0055
MQ c = 0.01	6.0128e-04	0.3276	0.0051	0.0051
MQ c = 1	4.5807e-10	0.0175	0.0076	0.0062
MQ c = 2	2.2615e-13	0.0227	0.0079	0.0065

TAB. 1. Comparison of uniform norm errors.

points have been chosen to minimise the interpolation errors for the harmonic functions, yet we see from results given in [7] that increasing the number of points in the distribution (which also increases the degree of the interpolating function) does not necessarily produce better accuracy. However, these point distributions when used for the multiquadric function provide consistently better accuracy. Further evidence suggests that points considered optimal for the spherical harmonics are also 'good' for the multiquadric function when compared to an equal number of generally scattered points. However, this is due to the uniformity of the point distributions and similar results can be obtained on a refined icosahedral mesh.

Method	12 pts	92 pts	362 pts
Renka	0.1730	0.0103	0.8230e-03
MQ c = 0.01	0.2596	0.0170	0.0020
MQ c = 1	0.0715	7.7662e-05	1.9678e-10
MQ c = 2	0.0442	3.8206e-05	3.4113e-11

TAB. 2. Multiquadric vs Renka for $f(x,y,z) = \sin(x+y) + \sin(xz)$.

The Renka algorithm produced similar results to those obtained using the multiquadric (for small c) for the F3 and F4 functions, although the results for the functions F1 and F2 were poor. Further comparisons with the Renka algorithm have been made using 12, 92 and 362 icosahedral points to interpolate the function $f(x,y,z) = \sin(x+y)+\sin(xz)$. The uniform norm interpolation errors have been calculated on the previously mentioned spherical cap. Again we see that the multiquadric function produces better accuracy than the Renka method when the number of interpolation points is increased.

5 Evolution of a smooth closed surface

In this section we return to the local interpolation scheme of §3 and apply it to scattered data on a smooth closed surface. This is the setting described in [8], where initially the interface is spherical with the point locations determined by subdivision of an icosahedral mesh. Each set of points consists of a central point together its nearest neighbours, giving sets of 6 points associated with the 12 vertices of the icosahedron and sets of 7 points otherwise. The local method of Renka [5] is followed and, for a chosen point, a local coordinate system is defined with this point on the z-axis. The local point set is projected onto the xy-plane and the surface heights provide the data values. This typically gives a configuration very close to the hexagon points (3.1) with an additional point at the centre, except for those points associated with the icosahedron vertices where the arrangement is a pentagon. As the iscosahedral mesh is refined these configurations become less regular.

The addition of the central point to the hexagon points increases the order of the approximation. When the surface is spherical, the symmetry of the data ensures that the computed unit normal at the centre point for polynomial, MQ or TPS is exact except for rounding error (*e.g.* for MQ the error is $||n - n_{MQ}||_2 = 3 \times 10^{-14}$). However, taking MQ with $c = 10$ and a sphere of radius 9, if the central point is displaced from the origin to (0.01,0.01) the error in the normal is 3×10^{-3}. To illustrate convergence for an irregular point set, the hexagon points are perturbed by the addition of a factor $(i-1)\epsilon h[1,1]^T$ for points $i = 1, 2 \ldots, 6$ with h the radius of the circumcircle and taking $\epsilon = 0.05$. For MQ with $c = 10$, the error in the surface normal is $O(h^3)$ whereas, for $c = 0.4$, the error is larger and the rate of convergence varies (see Table 3).

h	$\|\|n - n_{MQ}\|\|_2$, $c = 10$	$\|\|n - n_{MQ}\|\|_2$, $c = 0.4$
1.0	3.15×10^{-5}	6.14×10^{-3}
0.5	3.85×10^{-6}	1.26×10^{-3}
0.1	3.06×10^{-8}	6.35×10^{-6}
0.05	4.99×10^{-9}	8.47×10^{-7}

TAB. 3. Error in MQ approximation to surface normal of sphere, irregular point set.

Accurate curvature values are essential for an interface which is driven by surface tension. The exact value of $\kappa = -2/9$ for a sphere of radius 9, together with the computed values, are shown in Table 5. The polynomial and MQ with $c = 10$ are close to the exact value.

Method	κ
exact	-0.222...
polynomial	-0.222912
MQ c = 0.1	-1.638002
MQ c = 10.0	-0.225387

TAB. 4. Curvature, $\kappa = 2H$, evaluated at the central point of a regular hexagon.

It is found that, for the icosahedral mesh with $N = 362$, the local point sets are sufficiently regular to give good accuracy for surface normals and curvature using MQ interpolants when c is chosen to be 'large' in relation to the point spacing. This mesh also gives a corresponding accuracy for the discretised integral equation. These points can thus be considered 'good' for the MQ approximation. However, if the mesh is further refined or the surface deforms during its evolution, then the approximation becomes 'less good' as the regularity of the point locations is lost. Numerical experiments suggest second order convergence with point separation for irregular local point sets.

6 Conclusions

The behaviour of MQ and TPS interpolants can be interpreted by reference to the corresponding 'least' polynomial interpolant, with the MQ connecting the polynomial C^∞ surface to the tensioned surface of the TPS as the parameter c decreases. The MQ interpolant with 'large' c (relative to the point separation) exhibits the properties of the polynomial case and is similarly affected by the location of data points. Thus, points on a circle in the plane can be 'good' if the function to be represented is harmonic, but in general give only first order convergence on the interior. For data on the sphere, 'good' points for polynomial interpolation are also good for the MQ with 'large' c, but other near equispaced point distributions appear to give similar accuracy with MQ. The tensioning effect of smaller values of c can improve the results if the underlying function is not C^∞. When applied to an evolving interface, starting from an initially spherical shape and a refined icosahedral point distribution, it is found that local MQ approximations to the surface derivatives are affected by the point locations. This can be understood by reference to the polynomial interpolant to data located on a circle and causes an irregularity in the convergence as N increases.

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